

based" machines) has a machine-language instruction named (MOVE and EDIT, which permits a considerable variety of editing features at hardware speeds. This suggests that a moderate programming modification could enable the full power of the EDIT instruction to be added to the FORTRAN language for such a computer. The author has, in fact, done this for Version 4 of 1410 FORTRAN. From the user's standpoint, the extension takes the form of a new specification type in the FORMAT statement, allowing a "pictorial", reminiscent of the COBOL "picture." This pictorial (which is practically identical with the corresponding 1410 machine language specification) is effective only with the "F" and "I" output modes.

As an example, we can write in a 1410 FORTRAN program:

```
WRITE OUTPUT TAPE 6, 100, A, B, K
100 FORMAT (F(XX$0.XX), F6.2, I(XX.XX))
```

This results in the following 1410 treatment:

	Internal	Specification	1410 Edit Word	Output
A	100.0	F(XX\$0.XX)	bb\$0.bb	\$100.00
B	100.0	F6.2	None	100.00
K	100	I(XX.XX)	bb.bb	1.00

where the b's represent blanks. We have substituted X's for the blanks in the source format as a documentation aid. For further examples of 1410 hardware editing see page 38 of the IBM 1410 Reference Manual, Form No. A22-1407-2.

To create this feature in the 1410 FORTRAN all formats are examined at execution time for edit-type specifications. When an edit-type specification is encountered, it is converted to a standard edit word and placed in the I/O buffer. After the data word has been arranged for printing it is edited into this standard edit word. All checking features of the 1410 IO COMMON package are utilized. Fixed-point variables are edited directly from location 0500. Converted f-fields are moved to a new area by the standard IO COMMON package from which they are edited. The standard features of the original 1410 IO Common package are not disturbed.

This editing ability in 1410 FORTRAN allows business data processing problems to be compiled without losing either the facilities of the hardware edit feature or the programming advantages of FORTRAN. The author will be glad to supply the listing of this modification upon request.

Thanks are due F. J. Balint and E. B. Weinberger for suggestions leading to this work and to Dr. Weinberger for a number of programming suggestions.

JOHN E. FEDAKO

Gulf Research & Development Company
Pittsburgh, Pennsylvania

LETTER TO THE EDITOR

On the Communications Index

Dear Editor:

I have found the "Index to the Communications of the ACM, Volumes 1-5" the March issue of *Communications* extremely useful. I am sure that other members have found the index equally useful and I would like to add my appreciation to Mr. Youden of NBS for a job well done.

Perhaps all ACM members have not noticed that the index may be easily detached from the issue by simply removing the binding staples. Because of the method of binding the index into the issue this results in a conveniently folded section which carries its own staples.

C. L. McCARTY, JR.
Editor, Techniques Department
Communications of the ACM



J. WEGSTEIN, Editor

ALGORITHM 173

ASSIGN

OTOMAR HÁJEK

Research Institute of Mathematical Machines, Prague,
Czechoslovakia

procedure *assign* (*a*) the value of : (*b*) with dimension : (*dim*)
indices : (*ind*) bounds : (*low*, *up*) tracer : (*j*);

value *dim*; **integer** *dim*, *ind*, *low*, *up*, *j*;

comment This procedure uses Jensen's device (cf. ALGOL Report, procedure Innerproduct) twice: the *a*, *b* may depend on *ind* and also *ind*, *low*, *up* may depend on *j*;

begin

j := *dim*;

for *ind* := *low* **step** 1 **until** *up* **do**

if *dim* > 1

then

begin

assign (*a*, *b*, *dim*-1, *ind*, *low*, *up*, *j*);

j := *dim*

end

else *a* := *b*

end *assign*;

comment The obvious use of "assign" is in assigning the value of one array to another. The point here is that one procedure declaration serves for all the dimensions used. In fact, the dimension may even be a variable: thus a procedure essentially identical with "assign" was used by the author in implementing the recursive own process in an ALGOL compiler.

However, in addition to this, "assign" can have further functions, as illustrated below. The activation *assign* (*a*, (if *i*=1 **then** **false** **else** *a*) $\forall b_{i,i}, 1, i, 1, n, j$) will calculate the join-trace of a Boolean 2-dimensional array *b*.

assign (*a*_{*i*1,*i*2}, (if *i*₃=1 **then** 0 **else** *a*_{*i*1,*i*2}) + *b*_{*i*1,*i*3} × *c*_{*i*3,*i*2}, 3, *i*₃, 1, if *j* = 1 **then** *n* **else** if *j* = 2 **then** *m* **else** *p*, *j*)

will assign to *a* the matrix product of *b*, *c*. It may be noticed that, more generally, "assign" will perform all the tensor operations, e.g. tensor multiplication, alternation, etc.

ALGORITHM 174

A POSTERIORI BOUNDS ON A ZERO OF A POLYNOMIAL*

ALLAN GIBB

University of Alberta, Calgary, Alberta, Canada

comment The procedures below make use of Algorithm 61, Procedures for Range Arithmetic [*Comm. ACM* 4 (1961)]. It is assumed that the procedures below and the range arithmetic procedures are contained in an outer block and, therefore, that the procedures are available as required. Together the procedures make possible an attempt to determine absolute bounds

* These procedures were developed under Office of Naval Research Contract Nonr-225(37) at Stanford University. The author wishes to thank Professor George E. Forsythe for assistance with this work.

on a zero of a polynomial given an initial estimate of the zero. The procedures below are given for the complex case but may readily be adapted for the real case;

```

procedure RngPlyC (N, A, Z, P);
comment RngPlyC finds bounds [P1, P2] + i[P3, P4] on the
value of an nth degree polynomial  $\sum_{k=0}^n \{[a_{4k+1}, a_{4k+2}] + i[a_{4k+3}, a_{4k+4}]\} z^k$  with complex range coefficients for a complex range argument  $z = [Z1, Z2] + i[Z3, Z4]$ ;
integer N; array A, Z, P;
begin integer K, J; array X, Y[1 : 4];
P[1] := P[2] := P[3] := P[4] := 0;
for K := 4 × N step -4 until 0 do
  begin for J := 1 step 1 until 4 do X[J] := A[K+J];
  RNGMPYC (P[1], P[2], P[3], P[4], Z[1], Z[2], Z[3], Z[4], Y[1],
Y[2], Y[3], Y[4]);
  RNGSUMC (Y[1], Y[2], Y[3], Y[4], X[1], X[2], X[3], X[4],
P[1], P[2], P[3], P[4])
  end
end;
procedure RngAbsC (A, C);
comment RngAbsC produces the range absolute value [C1, C2]
of the complex range number [A1, A2] + i[A3, A4];
array A, C;
begin array B[1 : 4];
RANGESQR (A[1], A[2], B[1], B[2]);
RANGESQR (A[3], A[4], B[3], B[4]);
RANGESUM (B[1], B[2], B[3], B[4], C[1], C[2]);
C[1] := sqrt(C[1]);
C[2] := sqrt(C[2]);
comment It is assumed that the accuracy of the sqrt routine
used is known and that the maximum error in sqrt(C) is ± K
× CORRECTION(C). K is to be replaced below by its appropriate
numerical value;
C[1] := C[1] - K × CORRECTION (C[1]);
C[2] := C[2] + K × CORRECTION (C[2])
end;
procedure BndZrPlyC (N, ZOR, ZOJ, A, W);
integer N; real ZOR, ZOJ; array A, W;
comment BndZrPlyC attempts to determine bounds [W1, W2]
+ i[W3, W4] on a zero of an N-th degree polynomial in z with
complex range coefficients. It is assumed that an estimate
ZO = ZOR + iZOJ of the zero is available. The following
theorem is used. Assume f is regular at z0 with f'(z0) ≠ 0. Let
h0 = -f(z0)/f'(z0), let Δ be the region |z - z0| ≤ r |h0|, and
assume that f is regular in Δ. If, for some r > 0, |f'(z)| ≥ (1/r)
|f'(z0)| for all z ∈ Δ then Δ contains a zero of f (see [1], pp. 29-31);
begin integer I, J; array B[1:4×N], E, F, FP, D[1:4], AF,
AFP, G[1:2];
real RH, RHS, NL, NR, R, RNL, RNR;
for I := 1 step 1 until N do
  begin J := 4 × I;
  RANGEMPY (I, I, A[J+1], A[J+2], B[J-3], B[J-2]);
  RANGEMPY (I, I, A[J+3], A[J+4], B[J-1], B[J])
  end;
  E[1] := E[2] := ZOR; E[3] := E[4] := ZOJ;
  RngPlyC(N, A, E, F);
  RngAbsC(F, AF);
  RngPlyC(N-1, B, E, FP);
  RngAbsC(FP, AFP);
  RANGEDVD(AF[1], AF[2], AFP[1], AFP[2], NL, NR);
  R := 2;
  1: RANGEMPY(R, R, NR, NR, RNL, RNR);
  RANGESUM(ZOR, ZOR, -RNR, RNR, W[1], W[2]);
  RANGESUM(ZOJ, ZOJ, -RNR, RNR, W[3], W[4]);
  comment We have replaced the disk of the theorem by a square;
  RngRlyC(N-1, B, W, D);
  RngAbsC(D, G);
  if G[1] = 0 then go to failure1;

```

```

comment failure1 and failure2 are non-local labels;
RANGEDVD(AFP[2], AFP[2], R, R, RH, RHS);
if G[1] < RHS then
  begin R := 2 × R;
  if R > 1024 then go to failure2;
  go to 1
  end
end

comment The following procedure may replace BndZrPlyC
above;
procedure BndZrPlyC2 (N, ZOR, ZOJ, A, W);
integer N; array A, W; real ZOR, ZOJ;
comment BndZrPlyC2 is similar to BndZrPlyC above. The
theorem used here follows. If, in the disk |z - z0| ≤ 2 |h0| we
have |f'(z)| ≤ |f'(z0)|/(2 |h0|), then there is a unique zero in
the disk (see [2], pp. 43-50);
begin integer I, J; array B[1:4×N], C[1:4×N-4], F, D, P,
S[1:4], X, T, Q, Y[1:2]; real V, VP, R, RL;
for I := 1 step 1 until N do
  begin J := 4 × I;
  RANGEMPY(I, I, A[J+1], A[J+2], B[J-3], B[J-2]);
  RANGEMPY(I, I, A[J+3], A[J+4], B[J-1], B[J])
  end;
for I := 1 step 1 until N - 1 do
  begin J := 4 × I;
  RANGEMPY(I, I, B[J+1], B[J+2], C[J-3], C[J-2]);
  RANGEMPY(I, I, B[J+3], B[J+4], C[J-1], C[J])
  end;
  D[1] := D[2] := ZOR;
  D[3] := D[4] := ZOJ;
  RngPlyC(N, A, D, F);
  RngPlyC(N-1, B, D, P);
  RngAbsC(F, T);
  RngAbsC(P, X);
  if X[1] = 0 then go to failure1;
  comment failure1 and failure2 are non-local labels;
  RANGEDVD(T[1], T[2], X[1], X[2], Q[1], Q[2]);
  RANGEMPY(2, 2, Q[2], Q[2], RL, R);
  RNGSUMC(-R, R, -R, R, ZOR, ZOR, ZOJ, ZOJ, W[1], W[2],
W[3], W[4]);
  RngPlyC(N - 2, C, W, S);
  RngAbsC(S, Y);
  RANGEDVD(X[1], X[1], R, R, V, VP);
  if Y[2] > V then go to failure2
end

```

References:

1. GIBB, ALLAN. ALGOL procedures for range arithmetic. Tech. Report No. 15, Appl. Math. and Statistics Laboratories, Stanford University (1961).
2. OSTROWSKI, A. M. *Solution of equations and systems of equations*. Academic Press, New York, 1960.

ALGORITHM 175

SHUTTLE SORT

C. J. SHAW AND T. N. TRIMBLE

System Development Corporation, Santa Monica, Calif.

```

procedure shuttle sort (m, Temporary, N);
value m; integer m; array N[1:m];
comment This procedure sorts the list of numbers N[1] through
N[m] into numeric order, by exchanging out-of-order number
pairs. The procedure is simple, requires only Temporary as
extra storage, and is quite fast for short lists (say 25 numbers)
and fairly fast for slightly longer lists (say 100 numbers). For

```

still longer lists, though, other methods are much swifter. The actual parameters for *Temporary* and *N* should, of course, be similar in type;

```

begin integer i, j;
for i := 1 step 1 until m - 1 do
  begin
    for j := i step -1 until 1 do
      begin
        if N[j] ≤ N[j+1] then go to Test;
      Exchange: Temporary := N[j]; N[j] := N[j+1];
                 N[j+1] := Temporary; end of j loop;
    Test: end of i loop
  end shuttle sort

```

ALGORITHM 176

LEAST SQUARES SURFACE FIT

T. D. ARTHURS

The Boeing Company, Transport Division, Renton, Wash.

```

procedure SURFIT (F, z, W, m, n) answers: (a, e, rms);
integer m, n; real rms; array F, z, W, e;
procedure Invert, sqrt;
comment Given a set of m ordinates and the corresponding
  values of n prescribed general functions, (fi), of one or more
  linearly independent variables, this procedure fits the points,
  in the least squares sense, with a function of the form  $a_1f_1 + a_2f_2 + \dots + a_nf_n$  where ai are the unknown coefficients. Also computed
  are the vectors of residuals (ej) and their lengths (rms).
  Provision is made for weighting the data points. Essentially,
  the matrix equation  $F^T W F a = F^T W z$  is solved, where a is the vector
  of unknowns, W is an  $m \times m$  diagonal matrix of data point
  weights, z is the vector of ordinate values and F is the
   $m \times n$  matrix of corresponding function values. The availability
  of a procedure Invert, which replaces a real matrix with
  its inverse, is assumed;
begin integer i, j, k; real sqsum, g; array G[1:n, 1:n];
comment G is working space for the inversion procedure;
sqsum := 0;
for i := 1 step 1 until n do
  for j := 1 step 1 until n do
    begin G[i, j] := 0;
      for k := 1 step 1 until m do
        G[i, j] := G[i, j] + F[k, i] × F[k, j] × W[k]
      end j;
    Invert (G, n);
  for i := 1 step 1 until n do
    begin a[i] := 0;
      for j := 1 step 1 until m do
        begin g := 0;
          for k := 1 step 1 until n do
            g := g + G[i, k] × F[j, k];
            a[i] := a[i] + g × z[j] × W[j]
          end k
        end j
      end i;
    for i := 1 step 1 until m do
      begin e[i] = y[i];
        for j := 1 step 1 until n do
          e[i] := e[i] - a[j] × F[i, j];
          sqsum := sqsum + e[i] ↑ 2
        end j;
      rms := sqrt (sqsum/m)
    end SURFIT

```

ALGORITHM 177

LEAST SQUARES SOLUTION WITH CONSTRAINTS

M. J. SYNGE

The Boeing Company, Transport Division, Renton, Wash.

```

procedure CONLSQ (A, y, w, n, m, r) results: (x) residuals:
  (e, rms);
real rms; integer n, m, r; array A, y, w, x, e; procedure
  abs, SURFIT;
comment This procedure solves an overdetermined set of n
  simultaneous linear equations in m unknowns,  $Ax = y$ . The
  first r equations ( $r \leq m$ ) are satisfied exactly and the remaining
   $n - r$  are satisfied as well as possible by the method of least
  squares. Each equation is assigned a weight from the vector w,
  although the first r weights have no relevance. This procedure
  may be used for curve or surface fitting when the approximating
  function or its derivatives are required to have fixed values at a
  number of points;
begin integer i, j, k, ii, ick; integer array ic[1:m];
array B[1:n-r, 1:m-r]; real Amax;
for i := 1 step 1 until r do
  begin k := 1; for j := 2 step 1 until m do
    begin if abs (A[i, j]) > abs (A[i, k]) then k := j; end;
    ic[i] := k; Amax := A[i, k]; for j := 1 step 1 until m do
      A[i, j] := A[i, j]/Amax; y[i] := y[i]/Amax;
    for ii := 1 step 1 until r do
      begin if ii = i then go to skip; Amax := A[ii, k];
        for j := 1 step 1 until m do
          A[ii, j] := A[ii, j] - A[i, j] × Amax;
          y[ii] := y[ii] - y[i] × Amax;
        skip: end ii
      end i;
      ick := r + 1; for j := 1 step 1 until m do
        begin k := 1;
          repeat: if j = ic[k] then go to next;
            k := k + 1; if r ≥ k then go to repeat;
            ic[ick] := j; ick := ick + 1;
          next: end k;
          for i := r + 1 step 1 until n do
            begin for k := 1 step 1 until r do
              y[i] := y[i] - y[k] × A[i, ic[k]];
              for j := r + 1 step 1 until m do
                begin B[i, j] := A[i, ic[j]];
                  for k := 1 step 1 until r do
                    B[i, j] := B[i, j] - A[i, ic[k]] × A[k, ic[j]]
                  end k
                end j
              end k;
              SURFIT (B, y[r+1:n], w[r+1:n], n - r, m - r, x[r+1:m],
                e[r+1:n], rms);
            comment The procedure SURFIT is called to solve the reduced
              set of  $n - r$  simultaneous linear equations in  $m - r$  unknowns,
               $Bx_2 = y_2'$ , which have no constraints;
            for j := r + 1 step 1 until m do x[ic[j]] := x[j];
            for j := 1 step 1 until r do
              begin x[ic[j]] := y[j];
                for i := r + 1 step 1 until m do
                  x[ic[j]] := x[ic[j]] - A[j, ic[i]] × x[ic[i]]
                end i
              end CONLSQ

```

ALGORITHM 178

DIRECT SEARCH

ARTHUR F. KAUPPE, JR.

Westinghouse Electric Corp., Pittsburgh, Penn.

```

procedure direct search (psi, X, DELTA, rho, delta, S);

```

```

value K, DELTA, rho, delta; integer K; array psi;
real DELTA, rho, delta; real procedure S;
comment This procedure may be used to locate the minimum
of the function S of K variables. A discussion of the use of this
procedure may be found in: Robert Hooke and T. A. Jeeves,
'Direct Search' Solution of Numerical and Statistical Problems
[J. ACM 8, 2 (1961), 212-229]. The notation is essentially that
used in Appendix B of the cited paper. The exceptions being the
spelling of the Greek letters and the introduction of notation to
distinguish between the process of calculating a value of S and
the value itself—thus S(phi) and Sphi. A modified version of this
procedure acceptable to the BAC compiler for the Burroughs
205 and 220 computers has been prepared and run successfully;
begin real SS, Spsi, Sphi, theta; array phi [1:K]; integer K, k;
procedure E; for k := 1 step 1 until K do
begin phi [k] := phi [k] + DELTA; Sphi := S(phi);
if Sphi < SS then SS := Sphi else
begin phi [k] := phi [k] - 2 × DELTA; Sphi := S(phi);
if Sphi < SS then SS := Sphi else phi [k] := phi [k] + DELTA
end E;
Start: Spsi := S(psi);
1: SS := Spsi;
for k := 1 step 1 until K do phi [k] := psi [k]; E;
if SS < Spsi then begin
2: for k := 1 step 1 until K do begin
theta := psi [k];
psi [k] := phi [k];
phi [k] := 2 × phi [k] - theta end;
Spsi := SS; SS := Sphi := S(phi); E;
if SS < Spsi then go to 2 else go to 1 end;
3: if DELTA ≥ delta then begin DELTA := rho × DELTA;
go to 1 end end

```

ALGORITHM 179 INCOMPLETE BETA RATIO* OLIVER G. LUDWIG

Mathematical Laboratory and Department of Theoretical Chemistry, University of Cambridge, England

* Based in part on work done at Carnegie Institute of Technology, Pittsburgh, Pennsylvania and supported by the Petroleum Research Fund of the American Chemical Society and by the National Science Foundation.

```

real procedure incompletebeta (x, p, q, epsilon);
value x, p, q; real x, p, q, epsilon;
begin real finsum, infsum, temp, temp 1, term, term 1, qrecur, index;
Boolean alter;
comment This procedure evaluates the ratio  $B_x(p, q)/B_1(p, q)$ ,
where  $B_x(p, q) = \int_0^x t^{p-1}(1-t)^{q-1} dt$ , with  $0 \leq x \leq 1$  and  $p, q > 0$ ,
but not necessarily integers. It assumes the existence of a non-
local label, alarm, to which control is transferred upon entry to
the procedure with invalid arguments. Also assumed is a proce-
dure to evaluate  $\int_0^\infty t^p e^{-t} dt$  which is called factorial(p), (cf. e.g.
Algorithm 80, March, 1962);
if  $x > 1 \vee x < 0 \vee p \leq 0 \vee q \leq 0$  then go to alarm;
if  $x = 0 \vee x = 1$  then begin incompletebeta := x; go to End end;
comment This part interchanges arguments if necessary to ob-
tain better convergence in the power series below;
if  $x \leq 0.5$  then alter := false else
begin alter := true; temp := p; p := q; q := temp; x :=
1 - x end;
comment This part recurs on the (effective) q until the power
series below does not alternate;

```

```

finsum := 0; term := 1; temp := 1 - x; qrecur := index := q;
for index := index - 1 while index > 0 do
begin qrecur := index;
term := term × (qrecur + 1) / (temp × (p + qrecur));
finsum := finsum + term
end;
comment This part sums a power series for non-integral effec-
tive q and yields unity for integer q;
infsum := term := 1; index := 0;
comment In the following statement the convergence criterion
might well be altered to term > epsilon, since infsum > 1 al-
ways, thus saving one divide per cycle at the cost, perhaps, of a
few more cycles;
for index := index + 1 while (term/infsum) > epsilon do
begin term := term × x × (index - qrecur) × (p + index - 1) /
(index × (p + index)); infsum := infsum + term
end;
comment This part evaluates most of the necessary factorial
functions, minimizing the number of entries into the factorial
procedure;
temp 1 := factorial (qrecur - 1);
term 1 := term 1 × factorial (qrecur + p - 1);
for index := qrecur step 1 until (q - 0.5) do
begin temp 1 := temp 1 × index;
term 1 := term 1 × (index + p)
end;
comment This part combines the partial results into the final
one;
temp :=  $x \uparrow p \times (\text{infsum} \times \text{term} / (p \times \text{temp}) + \text{finsum} \times \text{term} 1 \times$ 
 $(1 - x) \uparrow q / (q \times \text{temp} 1)) / \text{factorial}(p - 1)$ ;
incompletebeta := if alter then 1 - temp else temp;
end: end incompletebeta

```

ALGORITHM 180 ERROR FUNCTION—LARGE X HENRY C. THACHER, JR.*

Argonne National Laboratory, Argonne, Ill.

* Work supported by the U. S. Atomic Energy Commission.

```

real procedure erfL(x); value x; real x;
comment This procedure evaluates the error function of real
argument,  $\text{erf}(x) = (2/\sqrt{\pi}) \int_0^x e^{-u^2} du$  by the Laplace continued
fraction for the complementary error function:  $\text{erf}(x) = 1 -$ 
 $(1/(1+v/(1+2v/(1+3v/(1+\dots)))))/(\sqrt{\pi} x e^{x^2})$  where  $v = 1/$ 
 $(2x^2)$ . Successive even convergents of the continued fraction are
evaluated, using an algorithm suggested by Maehly, until the
full accuracy of the arithmetic being used is attained.
The continued fraction converges for all  $x > 0$ . For small  $x$ ,
however, convergence may be excessively slow, and overflow
may occur. In this region, the Taylor series converges satis-
factorily, and algorithms such as No. 123 are suitable.
For  $x \leq 0$ , the procedure calls the global procedure alarm.
The body of this procedure has been checked on the LGP-30
computer, using the Dartmouth Self Contained Algol Processor.
The program was used to tabulate  $\text{erf}(x)$  from 0.9(1)5.0. The
maximum error was  $2 \times 10^{-6}$ , which is explainable by roundoff
errors. The number of convergents calculated ranged from 36
for  $x = 0.9$  to 2 for  $x \geq 3.3$ . Overflow occurred for  $x = 0.87$ ;
begin integer m; real B min 2, B min 3, P, R, T, v, v 2;
if  $x \leq 0$  then alarm;
v :=  $x \times x$ ;
T :=  $-0.56418958/x/\exp(v)$ ;
comment The constant  $0.56418958 \dots = \pi^{-1/2}$ , and should
be given to the full accuracy required of the procedure;
v :=  $0.5/v$ ;

```

```

P = v × T;
v2 := v × v;
T := T + 1;
m := 0;
R := B min 3 := B min 2 := 1;
for m := m + 1 while T ≠ R do
  begin R := T;
    B min 3 := v × (m-1) × B min 3 + B min 2
    T := B min 2;
    B min 2 := v × m × B min 2 + B min 3;
    T := R - P/B min 2/T;
    P := m × (m+1) × v2 × P
  end while;
  erfL := T
end

```

ALGORITHM 181 COMPLEMENTARY ERROR FUNCTION— LARGE X

HENRY C. THACHER, JR.*

Argonne National Laboratory, Argonne, Ill.

* Work supported by the U. S. Atomic Energy Commission.

real procedure *erfcL*(x); **value** x; **real** x;
comment This procedure evaluates the complementary error function, $\text{erfc}(x) = 1 - \text{erf}(x) = (2/\sqrt{\pi}) \int_x^\infty \exp(-u^2) du$ by the Laplace continued fraction:

$$\text{erfc}(x) = (1/(1+v/(1+2v/(1+3v/(1+\dots)))))/(\sqrt{\pi} x e^{x^2})$$

where $v = 1/(2x^2)$. Successive even convergents of the continued fraction are evaluated, using an algorithm suggested by Maehly, until the full accuracy of the arithmetic being used is attained.

The continued fraction converges for all $x > 0$. For small x , however, convergence may be excessively slow, and overflow and round-off accumulation may occur. In this region, the Taylor series converges satisfactorily.

For $x \leq 0$, the procedure calls the global procedure *alarm*.

The body of this procedure has been checked on the LGP-30 Computer, using the Dartmouth Self Contained Algol Processor, for $x = 1.2(0.1)5.0$. Results were generally correct to 1 in the 6th significant digit, although a few errors were as large as 6 in that digit. The errors are believed to be due to round-off only. The number of convergents calculated ranged from 46 for $x = 1.2$ to 10 for $x = 5.0$.

Overflow occurred for $x = 1.183$;

```

begin integer m; real B min 2, B min 3, P, R, T, v, v2;
if x ≤ 0 then alarm;
v := x × x;
T := 0.56418958/x/exp(v);
comment The constant 0.56418958 ... =  $\pi^{-1/2}$ , and should be
given to the full accuracy required of the procedure;
v := 0.5/v;
v2 := v × v;
P := v × T;
m := R := 0;
B min 3 := B min 2 := 1;
for m := m + 2 while R ≠ T do
  begin R := T;
    B min 3 := v × (m-1) × B min 3 + B min 2;
    T := B min 2;
    B min 2 := v × m × B min 2 + B min 3;
    T := R - P/B min 2/T;
    P := m × (m+1) × v2 × P
  end while;
  erfc L := T
end

```

ALGORITHM 182

NONRECURSIVE ADAPTIVE INTEGRATION

W. M. McKEEMAN AND LARRY TESLER

Stanford University, Stanford, Calif.

```

real procedure Simpson(F) limits : (a, b) tolerance : (eps);
real procedure F; real a, b, eps; value a, b, eps;
begin comment A nonrecursive translation of Algorithm 145.
Note that the device used here can be used to simulate recursion
for a wide class of algorithms;
integer lvl;
switch return := r1, r2, r3;
real array dx, epsp, x2, x3, F2, F3, F4, Fmp, Fbp,
est2, est3 [1:30], pval[1:30, 1:3];
integer array rtrn [1:30];
real absarea, est, Fa, Fm, Fb, da, sx, est1, sum, F1;
comment the parameter setup for the initial call;
lvl := absarea := est := 0; da := b - a;
Fa := F(a); Fm := 4.0 × F((a+b)/2.0); Fb := F(b);
recur:
  lvl := lvl + 1; dx[lvl] := da/3.0;
  sx := dx[lvl]/6.0; Fl := 4.0 × F(a+dx[lvl]/2.0);
  x2[lvl] := a + dx[lvl]; F2[lvl] := F(x2[lvl]);
  x3[lvl] := x2[lvl] + dx[lvl]; F3[lvl] := F(x3[lvl]);
  epsp[lvl] := eps; F4[lvl] := 4.0 × F(x3[lvl]+dx[lvl]);
  Fmp[lvl] := Fm; est1 := (Fa+F1+F2[lvl]) × sx;
  Fbp[lvl] := Fb; est2[lvl] := (F2[lvl]+F3[lvl]+Fm) × sx;
  est3[lvl] := (F3[lvl]+F4[lvl]+Fb) × sx;
  sum := est1 + est2[lvl] + est3[lvl];
  absarea := absarea - abs(est) + abs(est1) + abs(est2[lvl]) +
abs(est3[lvl]);
if (abs(est-sum) ≤ epsp[lvl] × absarea) ∨ (lvl ≥ 30) then
begin comment done on this level;
  up : lvl := lvl - 1;
  pval[lvl, rtrn[lvl]] := sum;
  go to return [rtrn[lvl]]
end;
rtrn[lvl] := 1; da := dx[lvl]; Fm := F1;
Fb := F2[lvl]; eps := epsp[lvl]/1.7; est := est1;
go to recur; r1:
rtrn[lvl] := 2; da := dx[lvl]; Fa := F2[lvl];
Fm := Fmp[lvl]; Fb := F3[lvl]; eps := epsp[lvl]/1.7;
est := est2[lvl]; a := x2[lvl]; go to recur; r2:
rtrn[lvl] := 3; da := dx[lvl]; Fa := F3[lvl];
Fm := F4[lvl]; Fb := Fbp[lvl]; eps := epsp[lvl]/1.7;
est := est3[lvl]; a := x3[lvl]; go to recur; r3:
sum := pval[lvl, 1] + pval[lvl, 2] + pval[lvl, 3];
if lvl > 1 then go to up;
Simpson := sum
end Simpson

```

ALGORITHM 183

REDUCTION OF A SYMMETRIC BANDMATRIX TO TRIPLE DIAGONAL FORM

H. R. SCHWARZ

Swiss Federal Institute of Technology, Zürich, Switzerland

procedure *banded*(a, n, m);
value n, m; **integer** n, m; **array** a;
comment *banded* reduces a real and symmetric matrix of band type (order n, $a[i, k] = 0$ for $|i-k| > m$) by a sequence of orthogonal similarity transformations to triple diagonal form. The procedure represents a generalization of the algorithm m21 by H. Rutishauser. Due to symmetry only the upper part of the band matrix must be given and these elements are denoted for

convenience in the following way: $a[i, 0]$ ($i=1, 2, \dots, n$) represents the diagonal element in the i th row, and $a[i, k]$ ($i=1, 2, \dots, n-k$ and $k=1, 2, \dots, m$) represents the generally nonzero element in the i th row and the k th position to the right of the diagonal. After completion of the reduction, the elements of the symmetric triple diagonal matrix are given by $a[i, 0]$ ($i=1, 2, \dots, n$) and $a[i, 1]$ ($i=1, 2, \dots, n-1$);

```

begin integer  $r, k, i, j, p, rr$ ; real  $b, g, c, s, c2, s2, cs, u, v$ ;
for  $r := m \text{ step } -1 \text{ until } 2$  do
  begin
    for  $k := 1 \text{ step } 1 \text{ until } n-r$  do
      begin
        for  $j := k \text{ step } r \text{ until } n-r$  do
          begin
            comment This compound statement describes the rotation
              involving the  $i$ th and  $(i+1)$ st rows and columns
              in order to reduce either  $a[j, r]$  or the off-band element
               $g$  to zero, respectively. This rotation produces a new
              off-band element  $g$  (in general different from zero) provided
               $i + r < n$ ;
            if  $j = k$  then
              begin if  $a[j, r] = 0$  then go to endk;
                 $b := -a[j, r-1]/a[j, r]$ 
              end
            else
              begin if  $g = 0$  then go to endk;
                 $b := -a[j-1, r]/g$ 
              end;
               $s := 1/\text{sqrt}(1 + b \times b)$ ;  $c := b \times s$ ;
               $c2 := c \times c$ ;  $s2 := s \times s$ ;  $cs := c \times s$ ;
               $i := j + r - 1$ ;
            cross elements:
               $u := c2 \times a[i, 0] - 2 \times cs \times a[i, 1] + s2 \times a[i+1, 0]$ ;
               $v := s2 \times a[i, 0] + 2 \times cs \times a[i, 1] + c2 \times a[i+1, 0]$ ;
               $a[i, 1] := cs \times (a[i, 0] - a[i+1, 0]) + (c2-s2) \times a[i, 1]$ ;
               $a[i, 0] := u$ ;  $a[i+1, 0] := v$ ;
            column rotation:
              for  $p := j \text{ step } 1 \text{ until } i-1$  do
                begin
                   $u := c \times a[p, i-p] - s \times a[p, i-p+1]$ ;
                   $a[p, i-p+1] := s \times a[p, i-p] + c \times a[p, i-p+1]$ ;
                   $a[p, i-p] := u$ 
                end  $p$ ;
              if  $j \neq k$  then
                 $a[j-1, r] := c \times a[j-1, r] - s \times g$ ;
              row rotation:
                 $rr := \text{if } r \leq n-i \text{ then } r \text{ else } n-i$ ;
                for  $p := 2 \text{ step } 1 \text{ until } rr$  do
                  begin
                     $u := c \times a[i, p] - s \times a[i+1, p-1]$ ;
                     $a[i+1, p-1] := s \times a[i, p] + c \times a[i+1, p-1]$ ;
                     $a[i, p] := u$ 
                  end  $p$ ;
                if  $i+r < n$  then
                  new g: begin  $g := -s \times a[i+1, r]$ ;
                     $a[i+1, r] := c \times a[i+1, r]$ 
                  end
                end  $j$ ;
              endk: end  $k$ 
            end  $r$ 
          end  $r$ 
        end  $r$ 
      end  $r$ 
    end  $r$ 
  end  $r$ 

```

CERTIFICATION OF ALGORITHM 74 CURVE FITTING WITH CONSTRAINTS [J. E. Peck, *Comm. ACM*, Jan. 62]

KAZUO ISODA

Japan Atomic Energy Research Institute, Tokai, Ibaraki,
Japan

Algorithm 74 was hand-compiled into SOAP IIA for the IBM 650 and run successfully with no corrections except the case in which the origin (0, 0) are given as both a constraint and a sample.

CERTIFICATION OF ALGORITHM 123 REAL ERROR FUNCTION, $\text{ERF}(x)$ [Martin Crawford and Robert Techo, *Comm. ACM*, Sept. 1962]

HENRY C. THACHER, JR.*

Argonne National Laboratory, Argonne, Ill.

* Work supported by the U. S. Atomic Energy Commission.

The body of $\text{Erf}(x)$ was tested using the Dartmouth SCALP compiler for the LGP-30. For $x = 0(0.01)0.3$, the results agreed with tabulated values to 8 in the 7th decimal place, and for $x = 0.4(0.2)1.6$ the error was less than 1 in the 6th decimal. These results are compatible with the roundoff error in the arithmetic used. The computing time increased rapidly (by a factor of more than 10) as x increased from 0.01 to 1.6.

The following comments should be considered by users of the algorithm:

1. The parameter x should be called by value, both to allow the use of expressions, and also to avoid destruction of the actual parameter.
2. The constant $10-10$ in statement 2 determines the accuracy of the computation. Its value should be adjusted to the arithmetic being used, and the accuracy required. A machine-independent test could be made by substituting **if** $Y - T = Y$ **then** $\dots$.
3. For large x , the error function is more efficiently calculated from the Laplace continued fraction for $\text{erfc}(x)$. Algorithm 180 is based on this method.

A contribution to this department must be in the form of an Algorithm, a Certification, or a Remark. Contributions should be sent in duplicate to the Editor and should be written in a style patterned after recent contributions appearing in this department. An algorithm must be written in ALGOL 60 (see *Communications of the ACM*, January 1963) and accompanied by a statement to the Editor indicating that it has been tested and indicating which computer and programming language was used. For the convenience of the printer, contributors are requested to double space material and underline delimiters and logical values that are to appear in boldface type. Whenever feasible, Certifications should include numerical values.

Although each algorithm has been tested by its contributor, no warranty, express or implied, is made by the contributor, the Editor, or the Association for Computing Machinery as to the accuracy and functioning of the algorithm and related algorithm material, and no responsibility is assumed by the contributor, the Editor, or the Association for Computing Machinery in connection therewith.

The reproduction of algorithms appearing in this department is explicitly permitted without any charge. When reproduction is for publication purposes, reference must be made to the algorithm author and to the *Communications* issue bearing the algorithm.